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A NUMERICAL METHOD FOR THE RADIATION TRANSPORT EQUATION IN PLANE GEOMETRY

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1/3

A NUMERICAL METHOD FOR THE RADIATION TRANSPORT EQUATION IN PLANE GEOMETRY

I. INTRODUCTION

The scope of work reported here is the development of a numerical method for performing time dependent calculations of radiative energy transport through slabs is reported. Of guiding interest has been the retaining of contact with the diffusion approximation by maintaining a parallel of numerical methods. In doing so, it has been found that the radiation intensity may effectively be eliminated from the equations and from computer storage. As is the case in the diffusion approximation, only the material temperature remains. Conservation of energy is also a direct consequence of the method. However, to accomplish this objective a number of simplifications have been made which may limit the possibility of generalizing the method. These include the assumptions of:

1. Plane slab geometry and boundary conditions of several simple types.
   a. Free surface radiating into vacuum.
   b. Opaque surface with zero flux.
   c. Specified forward or backward flux into the slab.
2. Negligibility of the time for photon flight between emission and absorption. Related neglect of the specific heat of the radiation field in comparison with the specific heat of the material.
3. Local thermodynamic equilibrium of the material.
4. Interaction of radiation with material only through true absorption. No photon scattering. Frequency independent absorption coefficient.

Several of these assumptions, namely 2, 3, and neglect of scattering, may be satisfied by restricting consideration to low temperature transport through materials of not too small density. The more serious approximation of frequency independence of the absorption coefficient has been made in order to separate the two important problems of the geometrical behavior and the frequency behavior of the radiation transport equation. Extension of the present method to include groups of photons having different absorption coefficients will probably not offer serious difficulties to the present method. However, it is by no means clear that extension of this basic procedure to other geometries can be made. In this sense, the present work is of interest in its special applicability to slab problems. In compensation it offers a rather simple system of equations having small storage requirements and light stability restrictions which allow rapid solution of radiation transport problems.

II. INTEGRAL EQUATION FOR RADIATIVE TRANSFER

The assumptions of plane geometry and azimuthal symmetry of the radiation intensity permit considerable simplification of the equations of radiative transfer. As will be shown, the equation for the rate of change of material energy for this case can be reduced to an integral equation in which all reference to the intensity of the radiation field has been eliminated.

The equation for the rate of change of the intensity of the radiation field I_ν is:

$$\frac{\partial I_\nu}{c\partial t} + \mu \frac{\partial I_\nu}{\partial x} = \sigma_\nu' \left(\beta_\nu - I_\nu\right) \quad , \qquad (1)$$

where

$\mu = \cos \Theta$, Θ = polar angle of radiation,

$\sigma_\nu' = (1 - e^{-\frac{h\nu}{KT}})\,\sigma$, σ = absorption coefficient and σ_ν' takes account of the induced emission of the material.

$$B_\nu = \frac{2h}{C^3}\,\frac{\nu^3}{e^{h\nu/KT} - 1}$$

is the Planck function source assuming that the material collision rate is sufficient to establish local thermodynamic equilibrium in the material characterized by a material temperature T. Photon scattering and polarization are neglected in Equation (1).

Dropping the subscript indication of frequency and introducing the optical depth

$$\tau = \int_0^x \sigma' \, dx \quad ,$$

the intensity I at position τ and in direction μ can be expressed from Equation (1) in terms of the Planck function at points along the photon pencil of radiation:

$$I = e^{-\frac{\tau}{\mu}} \left[\frac{1}{\mu} \int_{\tau_0}^{\tau} B(\tau') \, e^{\frac{\tau'}{\mu}} \, d\tau' + I\,(\tau_0) \right] \qquad (2)$$

The effect of retardation or time of photon flight from the source has been neglected so that the intensity is approximated as depending only on instantaneous values of the Planck function. This corresponds to neglecting the first term of Equation (1) and is justified when the temperature waves travel much slower than c. The integral extends into the material to an arbitrary depth τ_0 at which point the intensity in the μ - direction is I (τ_0). This point may be taken as the boundary of the system or it might be a depth beyond which the contribution to I is negligible.

Having neglected the time dependence of the Boltzmann equation, the dependence on time of the radiation transport equation arises from the change of energy as governed by the first law of thermodynamics. In general, the total internal energy changes as a result of motion of the material and of entropy changing processes such as heat conduction. We wish to set in evidence in this discussion the characteristics of radiative transfer; consequently, we neglect all other mechanisms of energy change, including work, and write:

$$\frac{\partial E_M}{\partial t} = -\frac{\partial F}{\partial x} - \frac{\partial E_R}{\partial t} \quad , \tag{3}$$

where E_M is the material internal energy per unit volume, E_R is the radiant energy per unit volume given by:

$$E_R = 2\pi\int_0^\infty d\nu\int_{-1}^{1} I \, d\mu \quad ,$$

and

$$F = 2\pi c\int_0^\infty d\nu\int_{-1}^{1} I \, \mu d\mu \tag{4}$$

is the component of radiant energy flux along the x- direction. Since a numerical approach paralleling the diffusion treatment is ultimately desired, Equation (3) is integrated over a small interval to give the integral expression for energy conservation. Indeed, the integral equation could equally well have formed the starting point of the investigation. In the resulting conservative form the way to insure conservation of energy in the difference equation becomes clear. The desirability of this conservative property of the equations in fact dictates the choice of the following system over alternative forms based on the differential equation, Equation (3).

$$\frac{d}{dt}\int_{x_1}^{x_2} E_M \, dx = F(x_1) - F(x_2) \tag{5}$$

In the above we have neglected the rate of change of radiative energy in comparison with that of the material energy as is justified for low temperature interactions.

In order to remove the explicit appearance of I from Equation (4) for the fluxes, we use Equation (2) to obtain an integral expression in which the sources of radiation in the emission of the material are displayed. Forward and backward directions are treated separately: for the forward direction, $\mu > 0$, the integral extends from $\tau_0 = -\infty$ where $I(\tau_0) = 0$; for $\mu < 0$ we take $\tau_0 = +\infty$ and again assume $I(\tau_0) = 0$.

$$\int_0^1 I\,\mu d\mu = \int_{\infty}^{\tau} B\, d\tau' \int_0^1 e^{-\frac{\tau-\tau'}{\mu}}\, d\mu \quad ,$$

$$\int_{-1}^0 I\,\mu d\mu = \int_{\tau}^{\infty} B\, d\tau' \int_{-1}^0 (-1)\, e^{-\frac{\tau-\tau'}{\mu}}\, d\mu \quad . \tag{6}$$

The angular integrations in Equations (6) are particularly simple because the source B does not depend on the angle. Introducing the $E_n(x)$ functions[2] defined by:

$$E_n(x) = \int_0^1 e^{-\frac{x}{\mu}}\, \mu^{n-2}\, d\mu \quad ,$$

these expressions become:

$$\int_0^1 I\,\mu d\mu = \int_{-\infty}^{\tau} B(\tau')\, E_2(\tau - \tau')\, d\tau' \quad ,$$

$$\int_{-1}^0 I\,\mu d\mu = -\int_{\tau}^{\infty} B \cdot E_2(\tau' - \tau)\, d\tau' \quad . \tag{7}$$

Equation (5) becomes:

$$\frac{d}{dt}\int_{x_1}^{x_2} E_M\, dx = 2\pi c \int_0^{\infty} d\nu \Big[-\int_{-\infty}^{\tau_2} B \cdot E_2(\tau_2 - \tau')\, d\tau'$$

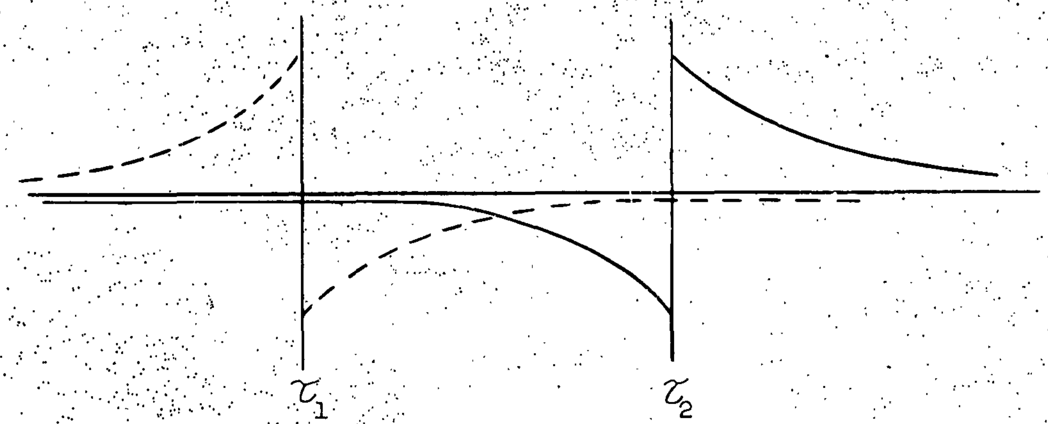
$$+ \int_{\tau_2}^{\infty} B \cdot E_2(\tau' - \tau_2)\, d\tau' \quad ,$$

$$+ \int_{-\infty}^{\tau_1} B \cdot E_2(\tau_1 - \tau')\, d\tau' - \int_{\tau_1}^{\infty} B \cdot E_2(\tau' - \tau_1)\, d\tau' \Big] \quad . \tag{8}$$

Equation (8) which is the starting point of the numerical work expresses the dependence of the rate of change of energy in the selected region on the attenuated sources as they compose the radiative fluxes. The appearance of E_2 functions instead of the exponential arises from weighting with more

[2] see, for example, Appendix A of "Introduction to the Theory of Neutron Diffusion" by K. M. Case, George Placzek, F. deHoffmann, Los Alamos Scientific Laboratory notes.

strongly attenuated oblique rays while the positive and negative terms correspond with forward and backward contributions to the flux integral. We illustrate the nature of the contributions to Equation (8) by schematically indicating the behavior of the kernels of the integrands.



For completeness, we return to the differential expression of Equation (3) to tabulate several alternative forms which may be of interest. Forming $\frac{\partial F}{\partial x} + \frac{\partial E_R}{\partial t}$ from Equation (4),

$$-\frac{\partial E_M}{\partial t} = \frac{\partial E_R}{\partial t} + \frac{\partial F}{\partial x} = 2\pi c \int_0^\infty d\nu \int_{-1}^{1} \left[\frac{\partial I}{c\,\partial t} + \mu \frac{\partial I}{\partial x}\right] d\mu$$

$$= 4\pi c \int_0^\infty \sigma' \, d\nu \int_{-1}^{1} I \, d\mu \quad , \tag{9}$$

in which Equation (1) has been used. Equation (9) expresses the statement that the rate of change of material energy is the difference between rates of absorption of I (which occurs only in the average intensity) Equation (2) for I is integrated separately in the forward and backward directions. Thus, the integrals contributing to E_R, similar to Equations (6), are:

$$\int_0^1 I \, d\mu = \int_{-\infty}^{\tau} B \cdot d\tau' \int_0^1 e^{-\frac{(\tau - \tau')}{\mu}} \frac{d\mu}{\mu} = \int_{-\infty}^{\tau} B \cdot E_1 (\tau - \tau') \, d\tau' \; ,$$

$$\int_{-1}^{0} I \, d\mu = \int_{\tau}^{\infty} B \cdot d\tau' \int_0^1 e^{-\frac{(\tau' - \tau)}{\mu}} \frac{d\mu}{\mu} = \int_{\tau}^{\infty} B \cdot E_1 (\tau' - \tau) \, d\tau' \; .$$

Using these results in Equation (9), the equation determining the temperature of the material is:

$$C_v \frac{dT}{dt} = 2\pi c \int_0^{\infty} \sigma \, d\nu \left[-2B(\tau) + \int_{-\infty}^{\infty} B(\tau') \, E_1 \, (|\tau - \tau'|) \, d\tau' \right] , \qquad (10)$$

where C_v is the specific heat at constant volume of the material and $B(\tau)$ depends on position through the temperature. Use of Equation (2) for I in which photon retardation has been neglected implies in Equation (10) that the energy in the radiation field must be small enough compared with that of the material to warrant omission from the energy equation. Equation (10) is a nonlinear integro-differential equation for the temperature containing no further reference to the radiation field intensities. The terms corresponding to the emission and absorption of energy by the material are displayed as the negative and positive members of Equation (10). The limiting case of optically thin material in a vacuum is given by the first term; the frequency integral of it gives the well known "Planck Mean Absorption Coefficient" which is frequently computed together with the Rosseland mean from absorption coefficient values.

The integral describing the contribution from absorption to the energy change in Equation (10) can be transformed through integration by parts.

$$\int_{-\infty}^{\infty} B(\tau') \, E_1 \, (|\tau - \tau'|) \, d\tau' = 2 \, B(\tau) + \int_{\tau}^{\infty} \frac{dB}{d\tau'} \, E_2 \, (\tau' - \tau) \, d\tau'$$
$$- \int_{-\infty}^{\tau} \frac{dB}{d\tau'} \, E_2 \, (\tau - \tau') \, d\tau' \; .$$

Substitution in Equation (10) gives the following alternative form:

$$C_v \frac{dT}{dt} = 2\pi c \int_0^\infty \sigma' \; d\nu \left[\int_\tau^\infty \frac{dB}{d\tau'} E_2 (\tau' - \tau) \, d\tau' \right.$$

$$\left. - \int_{-\infty}^{\tau} \frac{dB}{d\tau'} E_2 (\tau - \tau') \, d\tau' \right] \quad . \tag{11}$$

Further integration by parts in Equation (11) yields:

$$C_v \frac{dT}{dt} = 2\pi c \int_0^\infty \sigma' \; d\nu \int_{-\infty}^\infty \frac{d^2B}{d(\tau')^2} E_3 (|\tau - \tau'|) \, d\tau' \tag{12}$$

III. LIMITING EXPRESSIONS AND APPROXIMATIONS

Equation (12) is a convenient form to discuss the limiting case in which the temperature changes by a small amount within a mean-free path. Expansion of B'' (τ') about the point τ allows the evaluation of the leading term of the integral in Equation (12). The result is:

$$C_v \frac{dT}{dt} = \frac{4\pi c}{3} \int_0^\infty \sigma' \frac{d^2B}{d\tau^2} d\nu = \frac{4\pi c}{3} \frac{d}{dx} \int_0^\infty \frac{dB}{dx} \frac{d\nu}{\sigma'}$$

$$= \frac{4\pi c}{3} \frac{d}{dx} \left(\frac{dT}{dx} \int_0^\infty \frac{dB}{dT} \frac{d\nu}{\sigma'} \right) = \frac{ca}{3} \frac{d}{dx} \left(\frac{1}{\sigma_R} \frac{dT^4}{dx} \right) \quad , \tag{13}$$

where

$$\frac{1}{\sigma_R} = \frac{\int_0^\infty \frac{dB}{dT} \frac{d\nu}{\sigma'}}{\int_0^\infty \frac{dB}{dT} \, d\nu}$$

is the Rosseland mean-free path. Equation (13) gives the radiative diffusion approximation in which the energy of the radiation field has been neglected.

The optically thin result obtained from Equation (10) is the opposite extreme in approximation

$$C_v \frac{dT}{dt} = -\sigma_p \, ca \, T^4 \quad , \tag{14}$$

where

$$\sigma_p = \frac{\int_0^{\infty} B \, \sigma^{-1} \, d\nu}{\int_0^{\infty} B \, d\nu}$$

is the Planck mean absorption coefficient.

If the absorption coefficient depends on type of material, density and temperature but not on the frequency (the "gray atmosphere" approximation) the integration over frequency can be carried out in Equation (10):

$$C_v \frac{dT}{dt} = \sigma^{-1} \, ca \left[- T^4 (\tau) + \frac{1}{2} \int_{\infty}^{\infty} T^4 (\tau') \, E_1 (|\tau - \tau'|) \, d\tau' \right] . \tag{15}$$

The corresponding approximation to Equation (8) is obtained by using the following value of $F(x_j)$ in Equation (5):

$$F(x_j) = \frac{ca}{2} \left[\int_{\infty}^{\tau_j} T^4(\tau') \, E_2 \, (\tau_j - \tau') \, d\tau' - \int_{\tau_j}^{\infty} T^4(\tau') \, E_2 \, (\tau' - \tau_j) \, d\tau' \right] . \tag{16}$$

IV. DIFFERENCE EQUATIONS FOR RADIATION TRANSPORT

In formulating a suitable numerical approximation to Equation (5) we keep in mind several criteria. The method should

1. be as simple and easy to compute as possible
2. retain property of energy conservation
3. be sufficiently accurate to limit to the diffusion and transparent regimes properly
4. have an adequately wide region of numerical stability to permit fast integration forward in time.

In conformity with the radiation diffusion - hydrodynamics treatment, the region of interest is divided into a limited number of adjacent slabs or zones. In each zone the characteristic temperature is chosen so that the corresponding specific energy when multiplied by the zone mass gives the correct total zone energy. As a first approach to this method, we devise a simple explicit treatment of the temperature. The time derivative of the material energy is written as:

$$\frac{m_{j+1/2}\, C^n_{vj+1/2}}{\Delta t}\left(T^{n+1}_{j+1/2} - T^n_{j+1/2}\right) , \tag{17}$$

an expression which permits the temperature to be explicitly determined when the right hand side of the equation is evaluated with quantities known at time n. The quantities $m_{j+1/2}, C_{vj+1/2}$ are the zone mass and specific heat. The latter quantity may depend on time through its temperature dependence. As indicated in a subsequent section, this formulation is expected to have conditional stability. There also will be errors of second order in the time interval as is the case in the corresponding explicit treatment of the radiation diffusion treatment.

In conformity with the third criterion above it is necessary to use some care in evaluating the integrals contributing to the radiation flux. In particular, the simplest scheme in which the source is taken to be constant in each zone does not limit properly to the diffusion expression. As would be expected from the fact that the diffusion flux is given as a first derivative, it is necessary in the zones immediately adjacent to the boundary at which the flux is evaluated to use a linear interpolation of the source strength. In zones farther away the criterion of simplicity suggests assumption of constant source strength for the "tail" of the integration. Since the independent variable in the flux integrals is the optical depth it is necessary to evaluate it at zone interfaces on each cycle of the calculation. At time n the depth is given simply by:

$$\tau_j = \sum_{i=1}^{j-1} \sigma'_{i+1/2}\, \Delta x_{i+1/2} , \tag{18}$$

in which σ' is evaluated from the zone temperatures $T^n_{i+1/2}$. The optical depth of the zone center is $\tau_{j+1/2} = 1/2\,(\tau_j + \tau_{j+1})$. Intervals $\Delta\tau_{j+1/2}$

in the optical depth in general are expected to depend on position requiring that the interpolation formula be correspondingly more general.

In evaluating $F(x_j)$ from Equation (16), the use of linear interpolation is restricted to the half-zone on either side of the zone interface. In this region the fourth power of the temperature is given by interpolation:

$$T^4 = \alpha_j + \beta_j (\tau - \tau_j)$$

where

$$\alpha_j = \frac{(\tau_j - \tau_{j-1})\, T^4_{j+1/2} + (\tau_{j+1} - \tau_j)\, T^4_{j-1/2}}{\tau_{j+1} - \tau_{j-1}} \tag{19}$$

$$\beta_j = \frac{2(T^4_{j+1/2} - T^4_{j-1/2})}{\tau_{j+1} - \tau_{j-1}}$$

Carrying out the integration introduces E_3 for the constant regions and both E_3 and E_4 for the linear regions. The first integral corresponding to the forward current in Equation (16) is given by the sum of three terms,

$$\begin{aligned} {}_1f_j &= \alpha_j \left[1/2 - E_3 (\tau_j - \tau_{j-1/2})\right] + \beta_j \left[-1/3 + E_4 (\tau_j - \tau_{j-1/2}) \right. \\ &\quad \left. + (\tau_j - \tau_{j-1/2})\, E_3 (\tau_j - \tau_{j-1/2})\right] , \\ {}_2f_j &= T^4_{j-1/2} \left[E_3 (\tau_j - \tau_{j-1/2}) - E_3 (\tau_j - \tau_{j-1})\right] , \\ {}_3f_j &= \sum_{-\infty}^{j-2} T^4_{i+1/2} \left[E_3 (\tau_j - \tau_{i+1}) - E_3 (\tau_j - \tau_i)\right] , \end{aligned} \tag{20}$$

corresponding to the linear region from τ_j to $\tau_{j-1/2}$, the constant temperature half-zone from $\tau_{j-1/2}$ to τ_{j-1}, and the remaining zones of constant temperature for $\tau \leq_{j-1}$.

The analogous set of three terms for the backward current

$$
\begin{aligned}
{}_1b_j &= \alpha_j \left[1/2 - E_3 (\tau_{j+1/2} - \tau_j) \right] \\
&+ \beta_j \left[1/3 - E_4 (\tau_{j+1/2} - \tau_j) - (\tau_{j+1/2} - \tau_j)\, E_3 (\tau_{j+1/2} - \tau_j) \right] , \\
{}_2b_j &= T^4_{j+1/2} \left[E_3 (\tau_{j+1/2} - \tau_j) - E_3 (\tau_{j+1} - \tau_j) \right] , \qquad (21) \\
{}_3b_j &= \sum_{i=j+1}^{\infty} T^4_{i+1/2} \left[E_3 (\tau_i - \tau_j) - E_3 (\tau_{i+1} - \tau_j) \right] ,
\end{aligned}
$$

are to be summed and subtracted from the forward current to form the net flux at the point τ_j. The complete difference equation for the temperature results

$$F_j = \frac{ca}{2} ({}_1f_j + {}_2f_j + {}_3f_j - {}_1b_j - {}_2b_j - {}_3b_j) , \qquad (22)$$

from substituting such expressions for the zone boundary fluxes in the energy Equation (5) of which Equation (17) is the approximation for the left hand side. This expression may be solved for $T^{n+1}_{j+1/2}$. All of the contributing terms are assumed to be functions of the known temperatures $T^{n}_{j+1/2}$ which may be replaced in storage by the newly calculated values at the advanced time. Consequently, the method may be termed "an explicit integral formulation of the time-dependent radiation transport equation".

Boundary conditions are derived by considering the flux expression. A free surface condition corresponds to setting the source to zero for all zones beyond the free interface. A "hot wall" boundary to simulate the problem of the development of the diffusion wave from a hot source corresponds to giving all zones beyond a given boundary the same temperature.

V. STABILITY OF THE DIFFERENCE EQUATIONS

The system of difference equations, Equation (5), with boundary conditions and initial conditions may be solved for the temperatures of the material in an explicit step-by-step numerical calculation to obtain the solution at any desired time. In addition to the question of the truncation error incurred in the numerical approximation the question of stability of the solution must also be raised. If small errors are introduced, perhaps through rounding of the numbers, it is necessary that the difference equations not amplify the errors without bound. It is frequently the case that an inequality must be satisfied restricting the size of the time step to insure the stability of the solution in this sense.

Investigation of stability of the nonlinear equation with boundary conditions is a job beyond the scope of this investigation. However, a more modest effort will indicate some of the practical limitations to be observed in the numerical work to follow. As is generally done in this situation, the equations are linearized and the Von Neumann criterion is invoked. Introducing the dependent variable $\Phi^n_{j+1/2} = (T^n_{j+1/2})^4$ the equations become linear with constant coefficients provided that the solution is restricted to small variations.

$$\left(\frac{\rho\, C_v\, \Delta X_{j+1/2}}{4(T^n_{j+1/2})^3\, \Delta t}\right)(\Phi^{n+1}_{j+1/2} - \Phi^n_{j+1/2}) = \frac{ca}{2}\Big\{{}_1f_j + {}_2f_j + {}_3f_j$$

$$- {}_1f_{j+1} - {}_2f_{j+1} - {}_3f_{j+1} - {}_1b_j - {}_2b_j - {}_3b_j + {}_1b_{j+1} + {}_2b_{j+1} + {}_3b_{j+1}\Big\} \tag{23}$$

The f's and b's are functions of the $\Phi^n_{i+1/2}$ in accordance with the explicit formulation of the system. Since these equations are now linear equations with (assumed locally) constant coefficients, they also have the same form as the equations governing propagation of small errors. The solution is assumed to have the form:

$$\Phi(\tau, t) = e^{ik\tau} e^{\alpha t} \tag{24}$$

in which the wave number k plays the role of a free parameter while α is to be determined. For stability

$$\left| e^{\alpha \Delta t} \right| \leq 1 \text{ for all } k \quad ,$$

since the above is the amplification factor of the solution in one-time interval.

In order to further simplify the analysis the mesh interval and absorption coefficient are assumed constant. Thus,

$$\Delta X_{i+1/2} = \Delta X \quad ,$$

$$\Delta \tau_{i+1/2} = \Delta \tau \equiv \Delta \text{ for all } i \quad ,$$

which permits some terms to drop out of the flux. Substituting the assumed solution Equation (24) into Equation (23) and dividing by $\Phi^n_{j+1/2}$ one obtains:

$$\gamma_{j+1/2} \left(e^{\alpha \Delta \tau} - 1 \right) = {}_1f'_j + {}_2f'_j + {}_3f'_j - {}_1b'_j - {}_2b'_j - {}_3b'_j$$

$$- {}_1f'_{j+1} - {}_2f'_{j+1} - {}_3f'_{j+1} + {}_1b'_{j+1} + {}_2b'_{j+1} + {}_3b'_{j+1} \qquad (25)$$

where

$$\gamma_{j+1/2} = \frac{C_v \, m_{j+1/2}}{2 \, ca \, (T_{j+1/2})^3 \, \Delta t}$$

$${}_1f'_j = \alpha'_j \left[1/2 - E_3 \left(\tfrac{\Delta}{2}\right) \right] + \beta'_j \left[-1/3 + E_4 \left(\tfrac{\Delta}{2}\right) + \left(\tfrac{\Delta}{2}\right) E_3 \left(\tfrac{\Delta}{2}\right) \right]$$

$${}_2f'_j = e^{-ik\Delta} \left[E_3 \left(\tfrac{\Delta}{2}\right) - E_3 (\Delta) \right]$$

$${}_3f'_j = \sum_{n=1}^{\infty} e^{-ik(n+1)\Delta} \left[E_3 (n\Delta) - E_3 (n+1) \Delta \right]$$

$$_1b_j' = \alpha_j' \left[1/2 - E_3\left(\frac{\Delta}{2}\right)\right] + \beta_j' \left[1/3 - E_4\left(\frac{\Delta}{2}\right) - \frac{\Delta}{2}\; E_3\left(\frac{\Delta}{2}\right)\right]$$

$$_2b_j' = E_3\left(\frac{\Delta}{2}\right) - E_3\,(\Delta)$$

$$_3b_j' = \sum_{n=1}^{\infty} e^{ikn\Delta} \left[E_3\,(n\Delta) - E_3\,(n+1)\,\Delta\right]$$

in which

$$\alpha_j' = 1/2\,(1 + e^{-ik\Delta}) \quad ,$$

$$\beta_j' = \frac{1}{\Delta}\,(1 - e^{-ik\Delta}) \quad .$$

Also

$$_1f_{j+1}' = e^{ik\Delta}\;{}_1f_j' \quad ; \quad {}_2f_{j+1}' = e^{ik\Delta}\;{}_2f_j' \quad ; \quad {}_3f_{j+1}' = e^{ik\Delta}\;{}_3f_j' \quad ,$$

$$_1b_{j+1}' = e^{ik\Delta}\;{}_1b_j' \quad ; \quad {}_2b_{j+1}' = e^{ik\Delta}\;{}_2b_j' \quad ; \quad {}_3b_{j+1}' = e^{ik\Delta}\;{}_3b_j' \quad .$$

Combining these terms and rearranging them

$$e^{\alpha\Delta t} = 1 - \frac{1}{\gamma_{j+1/2}} \left\{\frac{4}{\Delta}\,(1 - \cos k\Delta) \left[1/3 - E_4\left(\frac{\Delta}{2}\right) - \frac{\Delta}{2}\,E_3\,(\Delta)\right] - \sum\right\}, \quad (26)$$

where

$$\sum = -2 \sum_{n=1}^{\infty} \left[\cos kn\Delta - \cos k(n+1)\,\Delta\right] \left[E_3(n\Delta) - E_3(n+1)\,\Delta\right] \quad .$$

The terms in the summation can be reduced to a single integral by interchanging summation and integration.

$$\sum = \sum_{n=1}^{\infty} \int_0^1 \mu d\mu \left\{(1 - e^{-\frac{\Delta}{\mu}})\,(e^{ik\Delta} - 1)\; e^{n\Delta(ik - \frac{1}{\mu})} + (1 - e^{-\frac{\Delta}{\mu}})\,(e^{-ik\Delta} - 1)\; e^{-n\Delta(ik + \frac{1}{\mu})}\right\}$$

$$= \int_0^1 \mu d\mu \left\{ \frac{(1 - e^{-\frac{\Delta}{\mu}})(e^{ik\Delta} - 1)}{e^{-\Delta(ik - \frac{1}{\mu})} - 1} + \frac{(1 - e^{-\frac{\Delta}{\mu}})(e^{-ik\Delta} - 1)}{e^{\Delta(ik + \frac{1}{\mu})} - 1} \right\}$$

$$= -2\int_0^1 e^{-\frac{\Delta}{\mu}} \mu d\mu \left\{ \frac{\cos k\Delta\,(1 - \cos k\Delta)\sinh\frac{\Delta}{\mu} + \sin^2 k\Delta\,(\cosh\frac{\Delta}{\mu} - 1)}{\cosh\frac{\Delta}{\mu} - \cos k\Delta} \right\} .$$

The quantity $\sum$ is a function of the two dimensionless quantities $k\Delta$ and Δ in which $k\Delta$ plays the role of a parameter to be varied in order to find the least stable value.

First, stability is considered for the limiting case of $\Delta >> 1$ for which

$$\sum = -2\,(1 + 2\cos k\Delta)(1 - \cos k\Delta)\,E_3(\Delta), \quad \Delta >> 1 \quad .$$

In this case, $e^{\alpha\Delta t} \leq 1$ since $\left|\sum\right|$ is less than the first term insuring that the coefficient of $\frac{1}{\gamma_{j+1/2}}$ is positive. It is easy to see that the most stringent stability condition is realized when $k\Delta = (2n+1)\pi$, n = 0,1,2 ... for which

$$\frac{1}{\gamma_{j+1/2}}\left[\frac{4f(\Delta)}{\Delta} - 2\,E_3(\Delta)\right] \leq 1 \quad ,$$

where

$$f(\Delta) = 1/3 - E_4\left(\frac{\Delta}{2}\right) - \frac{\Delta}{2}\,E_3(\Delta) \quad .$$

For $\Delta >> 1$, $f(\Delta) = 1/3$ and $\sum \longrightarrow 0$ giving the limiting stability condition

$$\Delta t \leq \frac{3\,\rho\,C_v\,\Delta x^2\,\sigma}{8\,ca\,T^3} \quad , \quad \Delta >> 1 \quad . \qquad (27)$$

As is expected from the fact that the difference equation becomes just the explicit diffusion equation in this case, Equation (27) is the diffusion stability condition. In general, $f(\Delta)$ is smaller than 1/3 as shown in Figure 1. For $\Delta << 1$ an expansion of f yields:

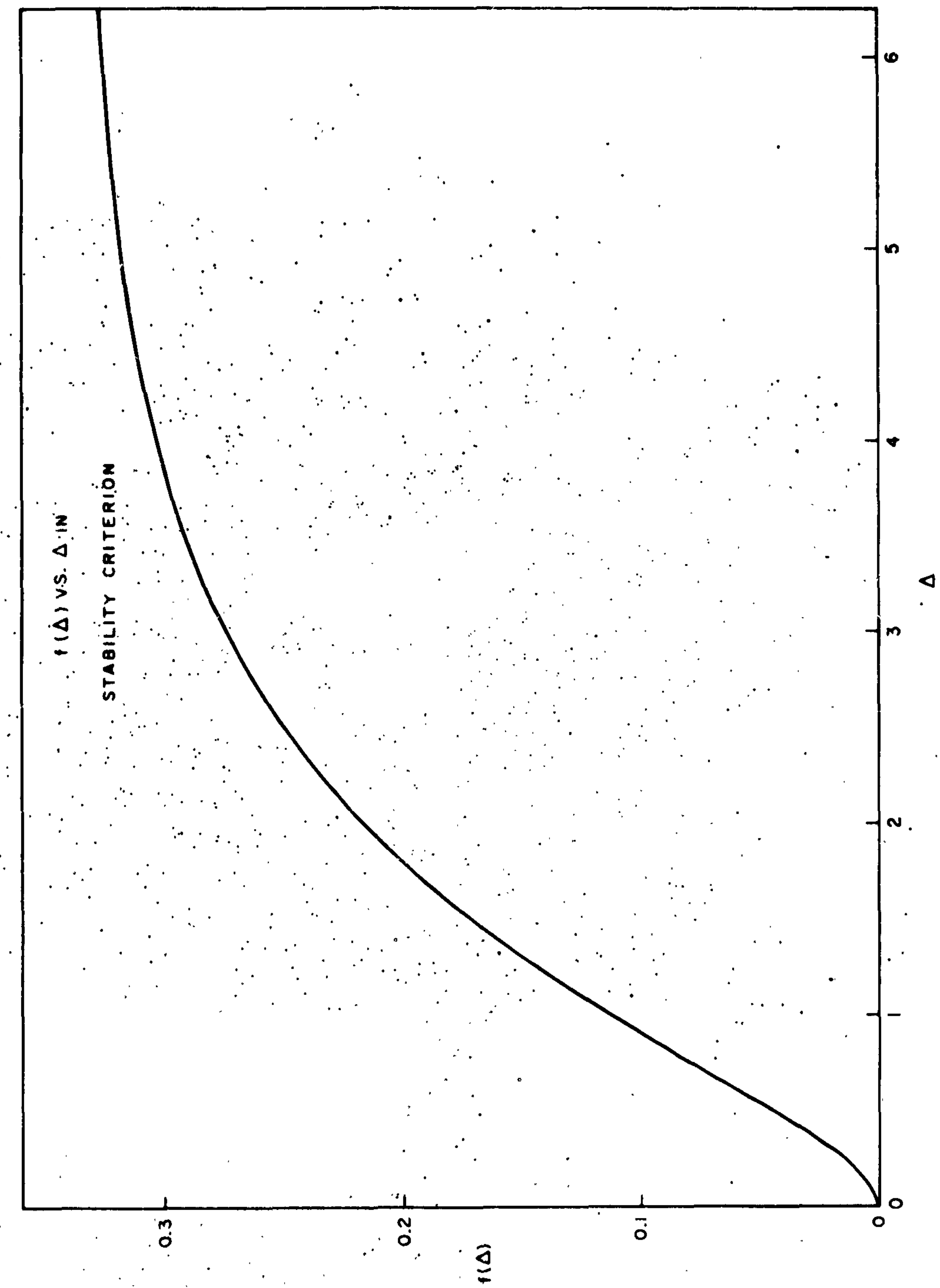


FIGURE I.

$$f \simeq \frac{3\Delta^2}{8} + \frac{11\Delta^3}{48} \ln(\gamma\Delta) \quad , \quad \Delta \ll 1$$

where

$$\ln \gamma = .5772 \quad .$$

Having obtained the stability condition for large Δ it is now necessary to investigate smaller values of Δ. In terms of defined quantities the amplification factor is:

$$e^{\alpha\Delta t} = 1 - \frac{1}{\gamma_{j+1/2}} \left[\frac{4}{\Delta} (1 - \cos k\Delta) \, f(\Delta) - \sum \right] \quad .$$

While, for large Δ, the term in $\sum$ could be neglected it must be considered in other cases. Some of the properties of $\sum$ are:

1. $\sum(2\pi n + k\Delta) = \sum(k\Delta)$, $n = 1,2,3 \ldots$

2. $\sum(2\pi - k\Delta) = \sum(k\Delta)$,

3. $\sum(k\Delta = 0) = 0$,

4. $\sum(k\Delta = \frac{\pi}{2}) = -2\int_0^1 e^{-\frac{\Delta}{\mu}} \dfrac{\cosh\frac{\Delta}{\mu} - 1}{\cosh\frac{\Delta}{\mu}} \mu d\mu < 0$,

5. $\sum(k\Delta = \pi) = 4\int_0^1 e^{-\frac{\Delta}{\mu}} \dfrac{\sinh\frac{\Delta}{\mu}}{\cosh\frac{\Delta}{\mu} + 1} \mu d\mu > 0$.

The stability behavior for $\Delta \ll 1$ is more complicated mathematically than the diffusion limit discussed above because $\sum$ contains the leading term in Equation (26). It is also true that $\sum$ does not take a simple limiting form in the neighborhood of $k\Delta = 0$. With neither a closed form expression for $\sum$ in the general case nor even one for $\Delta \ll 1$, the investigation has taken the form of evaluating integrals which bound $\sum$ from above and below. For $\Delta \ll 1$ the result of the bounding argument indicates that the coefficient of $\frac{1}{\gamma_{j+1/2}}$ remains positive, that it has a maximum value near $k\Delta = 0$, and that it rapidly falls to zero at $k\Delta = 0$. The stability condition,

$$\frac{\Delta}{\gamma_{j+1/2}} \leq 1 \quad , \quad \Delta \ll 1 \quad ,$$

gives the limiting time interval

$$\Delta t = \frac{\rho \, C_v}{2 \, \sigma \, ca \, T^3} \quad .$$

This value, depending not at all on the zone size Δx, is just the condition that the energy removed from an optically thin zone in the time interval not drive the material temperature negative enough to produce instability. The numerical value of the coefficient, however, depends on the linearization of the equations. A value representing the condition that the temperature in the actual equations must not become negative in a time step is:

$$\Delta t \leq \frac{\rho \, C_v}{\sigma \, ca \, T^3} \quad , \quad \Delta \ll 1 \quad , \tag{28}$$

which is to be preferred over the previous value.

As a basis for stability estimates to be tested with sample calculations the two limiting values given above are incorporated into a simple interpolation formula:

$$\frac{\sigma \, ca \, T^3 \, \Delta t}{\rho \, C_v} \leq 1 + \frac{3}{8} \Delta^2 \quad . \tag{29}$$

In an actual calculation in which the quantities entering Equation (29) depend on the zone, the minimum value of Δt resulting from testing all zones of the problem should be used to govern the time step.

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